



chain nodes :

12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 41
42 43 44 45 46

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 35 36 37 38 39 40

chain bonds :

1-12 2-13 3-17 4-16 5-14 7-12 8-21 9-20 10-19 10-23 11-18 14-15 21-22 23-24 23-25
25-26 26-27 27-28 28-29 28-30 30-31 31-32 32-33 32-34 34-35 36-41 40-42 41-43
41-44 42-45 42-46

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-11 7-8 8-9 9-10 10-11 35-36 35-40 36-37 37-38 38-39
39-40

exact/norm bonds :

1-2 1-6 1-12 2-3 2-13 3-4 3-17 4-5 4-16 5-6 7-12 7-11 7-8 8-9 9-10 9-20 10-11
10-19 11-18 14-15 21-22 23-24 23-25 25-26 26-27 27-28 28-29 32-33 32-34 34-35

exact bonds :

5-14 8-21 10-23 28-30 30-31 31-32 36-41 40-42 41-43 41-44 42-45 42-46

normalized bonds :

35-36 35-40 36-37 37-38 38-39 39-40

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom
40:Atom 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS